

Analytic Coulomb matrix elements in a three-dimensional geometry

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Using a complete basis set we have obtained an analytic expression for the matrix elements of the Coulomb interaction. These matrix elements are written in a closed form. We have used the basis set of the three-dimensional isotropic quantum harmonic oscillator in order to develop our calculations, which can be useful when treating interactions in localized systems.

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INTRODUCTION

Having an analytic expression for the Coulomb matrix elements is an important step for several numerical methods, like, for example, exact diagonalization method. In order to describe the Coulomb interaction in three dimensions, we have chosen the basis set of the isotropic harmonic oscillator for the single-particle wave functions, which, in one dimension, is written as

$$\psi_{n_x}(x) = (a\sqrt{\pi}2^{n_x}n_x!)^{-1/2} e^{-\frac{1}{2}x^2/a^2} H_{n_x}(x/a), \quad (1)$$

where $a = \sqrt{\hbar/m\omega}$ is taken as the characteristic unit length. One of the reasons for the election of this particular basis set is the Gaussian Product Theorem, which guarantees that the product of two Gaussian type orbitals (a linear combination of them in our case) centered on two different atoms is a finite sum of Gaussians centered on a point along the axis connecting them.

In previous works, several ways to evaluate the two-dimensional matrix elements using different approaches have been studied [1, 2, 3], such as restricting to the lowest Landau level due to simplicity reasons [4, 5].

The purpose of this paper is to report an analytic formula for the Coulomb interaction written in closed form. It can be easily implemented by computer means and could help to improve the performance of solid state simulations in which interactions are taken into account.

MATRIX ELEMENTS

In order to derive an analytical expression for the Coulomb interaction matrix elements we will proceed starting with the same approach as the one used in Ref. [6], i.e., writing the single-electron wave function and the Coulomb potential as their Fourier transform integrals:

$$\psi_{\lambda}(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int \phi_{\lambda}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{q}, \quad (2)$$

$$V(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \int \tilde{V}(\mathbf{q}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{q}, \quad (3)$$

where λ stands for a set of quantum numbers $\{n_i\}$ and $V(\mathbf{r}_1 - \mathbf{r}_2) = r_{12}^{-1}$ is the Coulomb potential. Now, the

two-particle matrix element, which, in real space is written as

$$\mathcal{V}_{\lambda_3\lambda_4}^{\lambda_1\lambda_2} = \int \psi_{\lambda_1}^*(\mathbf{r}_1) \psi_{\lambda_2}^*(\mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2) \times \psi_{\lambda_3}(\mathbf{r}_2) \psi_{\lambda_4}(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2, \quad (4)$$

is now expressed, in momentum space, as

$$\mathcal{V}_{\lambda_3\lambda_4}^{\lambda_1\lambda_2} = \frac{1}{(2\pi)^{3/2}} \int \phi_{\lambda_1}^*(\mathbf{q}_1) \phi_{\lambda_4}(\mathbf{q}_1 - \mathbf{q}) \times \phi_{\lambda_2}^*(\mathbf{q}_2) \phi_{\lambda_3}(\mathbf{q}_2 + \mathbf{q}) \tilde{V}(\mathbf{q}) d\mathbf{q}_1 d\mathbf{q}_2 d\mathbf{q}. \quad (5)$$

Eq. (5) can be rewritten in a more convenient and compact form. Let us define $C_{\lambda'}^{\lambda}(\mathbf{q})$ and $D_{\lambda'}^{\lambda}(\mathbf{q})$ as the following convolution integrals:

$$C_{\lambda'}^{\lambda}(\mathbf{q}) = \int \phi_{\lambda}^*(\mathbf{k}) \phi_{\lambda'}(\mathbf{k} - \mathbf{q}) d\mathbf{k} \quad (6)$$

$$= \int \psi_{\lambda}^*(\mathbf{r}) \psi_{\lambda'}(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r}, \quad (7)$$

$$D_{\lambda'}^{\lambda}(\mathbf{q}) = \int \phi_{\lambda}^*(\mathbf{k}) \phi_{\lambda'}(\mathbf{k} + \mathbf{q}) d\mathbf{k} \quad (8)$$

$$= \int \psi_{\lambda}^*(\mathbf{r}) \psi_{\lambda'}(\mathbf{r}) e^{i\mathbf{q}\cdot\mathbf{r}} d\mathbf{r} \quad (9)$$

$$= C_{\lambda'}^{\lambda}(-\mathbf{q}). \quad (10)$$

Substituting Eqs. (6) and (8) into Eq. (5) we obtain

$$\mathcal{V}_{\lambda_3\lambda_4}^{\lambda_1\lambda_2} = \frac{1}{(2\pi)^{3/2}} \int C_{\lambda_4}^{\lambda_1}(\mathbf{q}) D_{\lambda_3}^{\lambda_2}(\mathbf{q}) \tilde{V}(\mathbf{q}) d\mathbf{q}. \quad (11)$$

Now, it is straightforward to perform the integral appearing in Eq. (7) [7]. Using Cartesian coordinates, it is possible to separate all three variables and integrate independently. For simplicity reasons, let us integrate only along the x variable, the result then reads:

$$C_{n_x^+}^{n_x^-}(q_x) = \left(\frac{2^{n_x^+} n_{x-}^{14}!}{n_{x+}^{14}! 2^{n_x^+}} \right)^{1/2} i^{n_x^+ + n_x^4} (-1)^{n_x^4} \times e^{-q_x^2 a^2/4} \left(\frac{aq_x}{2} \right)^{|n_x^+ - n_x^4|} L_{n_{x-}^{14} - n_x^4}^{|n_x^+ - n_x^4|} (a^2 q_x^2/2), \quad (12)$$

where n_i^j is the quantum number referring to the i -axis of the particle j . We have also used the terms n_{i+}^{jk} and

n_{i-}^{jk} , which are defined as $\max(n_i^j, n_i^k)$ and $\min(n_i^j, n_i^k)$ respectively. The final form for $C_{\lambda_4}^{\lambda_1}(\mathbf{q})$ will be

$$C_{n_x^4 n_y^4 n_z^4}^{n_x^1 n_y^1 n_z^1}(\mathbf{q}) = \prod_{i \in \{x, y, z\}} C_{n_i^4}^{n_i^1}(q_i). \quad (13)$$

Using the relation between D and C shown in Eq. (10), it is trivial to find out the value of the former convolution integral.

It still remains to calculate the Fourier transform $\tilde{V}(\mathbf{q})$ of the spherically symmetric interaction potential $V(\mathbf{r})$.

$$\tilde{V}(q) = \sqrt{\frac{2}{\pi}} \frac{1}{q^2} \quad (14)$$

But it will be more convenient to substitute it by

$$\tilde{V}(q) = \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-(q_x^2 + q_y^2 + q_z^2)u} du \quad (15)$$

The integration over variables q_x , q_y and q_z can be performed all in the same fashion. Using the symmetry of the problem we only need to integrate over one variable, i.e. q_x and then use the same result for q_y and q_z . Therefore, integrating over q_x yields:

$$\int_{-\infty}^\infty e^{-(u+a^2/2)q_x^2} \left(\frac{aq_x}{2}\right)^{|n_x^1 - n_x^4| + |n_x^2 - n_x^3|} \times L_{n_{x-}^{14}}^{|n_x^1 - n_x^4|} (a^2 q_x^2 / 2) L_{n_{x-}^{23}}^{|n_x^2 - n_x^3|} (a^2 q_x^2 / 2) dq_x. \quad (16)$$

This integral does not vanish if and only if

$$|n_x^1 - n_x^4| + |n_x^2 - n_x^3| = 2s_x, \quad (17)$$

where $s_x = 0, 1, 2, \dots$. Therefore, using the previous selection rule and the power series for the associated Laguerre polynomial

$$L_n^l(x) = \sum_{k=0}^n \frac{1}{k!} \binom{n+l}{n-k} (-x)^k, \quad (18)$$

we can write Eq. (16) as

$$\sum_{k_x=0}^{n_{x-}^{14}} \frac{(-1)^{k_x}}{k_x!} \binom{n_{x+}^{14}}{n_{x-}^{14} - k_x} \sum_{k'_x=0}^{n_{x-}^{23}} \frac{(-1)^{k'_x}}{k'_x!} \binom{n_{x+}^{23}}{n_{x-}^{23} - k'_x} \times 2^{k_x + k'_x} \left(\frac{a}{2}\right)^{2s_x + 2k_x + 2k'_x} \times \frac{(2s_x + 2k_x + 2k'_x - 1)!!}{(2u + a^2)^{s_x + k_x + k'_x + 1/2}} \sqrt{2\pi}. \quad (19)$$

Taking into account only the u -dependent part in Eq. (19) and its symmetric extension for y and z variables, we end up with the last integral which will lead to the final result. This last integral is expressed as:

$$\int_0^\infty (2u + a^2)^{-\Omega - 3/2} du = \frac{1}{1 + 2\Omega} \frac{1}{a^{1+2\Omega}}, \quad (20)$$

where $\Omega = s_x + s_y + s_z + k_x + k_y + k_z + k'_x + k'_y + k'_z$.

Finally, collecting all the terms, we end up with the analytic expression for the Coulomb interaction matrix elements:

$$\begin{aligned} \mathcal{V}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2} &= \frac{1}{a} \sqrt{\frac{2}{\pi}} (-1)^{n_x^1 + n_y^1 + n_z^1 + n_x^4 + n_y^4 + n_z^4 - s_x - s_y - s_z} \\ &\quad \left(\frac{2^{n_{x+}^{14}} n_{x-}^{14}!}{n_{x+}^{14}!} \frac{2^{n_{y+}^{14}} n_{y-}^{14}!}{n_{y+}^{14}!} \frac{2^{n_{z+}^{14}} n_{z-}^{14}!}{n_{z+}^{14}!} \right)^{1/2} \left(\frac{2^{n_{x+}^{23}} n_{x-}^{23}!}{n_{x+}^{23}!} \frac{2^{n_{y+}^{23}} n_{y-}^{23}!}{n_{y+}^{23}!} \frac{2^{n_{z+}^{23}} n_{z-}^{23}!}{n_{z+}^{23}!} \right)^{1/2} \\ &\quad \sum_{k_x=0}^{n_{x-}^{14}} \frac{(-1)^{k_x}}{k_x!} \binom{n_{x+}^{14}}{n_{x-}^{14} - k_x} \sum_{k'_x=0}^{n_{x-}^{23}} \frac{(-1)^{k'_x}}{k'_x!} \binom{n_{x+}^{23}}{n_{x-}^{23} - k'_x} \frac{(2s_x + 2k_x + 2k'_x - 1)!!}{2^{2s_x + k_x + k'_x}} \\ &\quad \sum_{k_y=0}^{n_{y-}^{14}} \frac{(-1)^{k_y}}{k_y!} \binom{n_{y+}^{14}}{n_{y-}^{14} - k_y} \sum_{k'_y=0}^{n_{y-}^{23}} \frac{(-1)^{k'_y}}{k'_y!} \binom{n_{y+}^{23}}{n_{y-}^{23} - k'_y} \frac{(2s_y + 2k_y + 2k'_y - 1)!!}{2^{2s_y + k_y + k'_y}} \\ &\quad \sum_{k_z=0}^{n_{z-}^{14}} \frac{(-1)^{k_z}}{k_z!} \binom{n_{z+}^{14}}{n_{z-}^{14} - k_z} \sum_{k'_z=0}^{n_{z-}^{23}} \frac{(-1)^{k'_z}}{k'_z!} \binom{n_{z+}^{23}}{n_{z-}^{23} - k'_z} \frac{(2s_z + 2k_z + 2k'_z - 1)!!}{2^{2s_z + k_z + k'_z}} \\ &\quad \frac{1}{1 + 2(s_x + s_y + s_z + k_x + k'_x + k_y + k'_y + k_z + k'_z)}. \end{aligned} \quad (21)$$

RECURRENCE

Due to the six summatories appearing in Eq. (21), if the indices start to grow to values say, just of the order of tenths, the process for calculating a single matrix element can be quite time-consuming, and thus, a real bottleneck for any numerical simulation. Using the recurrence relations that the Hermite polynomials obey, it is possible to find a simple iterative formula for the matrix elements which will accelerate the process of calculating the matrix elements.

Let $\{n_-, n_+\}$ be any pair of quantum numbers $\{n_{i-}^{jk}, n_{i+}^{jk}\}$ with $i \in \{x, y, z\}$ and $jk \in \{14, 23\}$, satisfying $n_+ \geq n_-$. Then, the Coulomb matrix elements will satisfy (remaining indices omitted for clarity)

$$\begin{aligned} \mathcal{V}_{n_-}^{n_+} = & \sqrt{\frac{n_+ + 1}{n_-}} \mathcal{V}_{n_- - 1}^{n_+ + 1} + \sqrt{\frac{n_+}{n_-}} \mathcal{V}_{n_- - 1}^{n_+ - 1} \\ & - \sqrt{\frac{n_- - 1}{n_-}} \mathcal{V}_{n_- - 2}^{n_+}, \end{aligned} \quad (22)$$

for $n_- > 0$. If we consider the unnormalized matrix elements

$$\begin{aligned} \bar{\mathcal{V}}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2} = & \prod_{i \in \{1, 2, 3, 4\}} (2^{n_x^i} n_x^i! 2^{n_y^i} n_y^i! 2^{n_z^i} n_z^i!)^{\frac{1}{2}} \\ & \times \mathcal{V}_{n_x^3 n_y^3 n_z^3 n_x^4 n_y^4 n_z^4}^{n_x^1 n_y^1 n_z^1 n_x^2 n_y^2 n_z^2}, \end{aligned} \quad (23)$$

Eq. (22) can be transformed to

$$\bar{\mathcal{V}}_{n_- + 1}^{n_+} = \bar{\mathcal{V}}_{n_-}^{n_+ + 1} + 2n_+ \bar{\mathcal{V}}_{n_-}^{n_+ - 1} - 2n_- \mathcal{V}_{n_- - 1}^{n_+}. \quad (24)$$

Another interesting recurrence relation which, this time involves four indices $\{0, n_+\}$ and $\{m_-, m_+\}$, is the following

$$\bar{\mathcal{V}}_{0, m_-}^{n_+, m_+ + 1} = \bar{\mathcal{V}}_{0, m_-}^{n_+ + 1, m_+} + \bar{\mathcal{V}}_{0, m_- - 1}^{n_+, m_+}. \quad (25)$$

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